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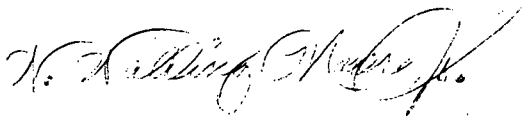
A MODIFIED QUADRUPOLE MASS SPECTROMETER  
WITH CUSTOM RF LINK RODS DRIVER FOR  
REMOTE OPERATION

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16. ABSTRACT  A commercial quadrupole residual gas analyzer (RGA) system has been upgraded for operation at extended cable lengths. Operation inside a vacuum chamber for the standard quadrupole nude head is limited to approximately 2 m from its externally located rf/dc generator because of the detuning of the rf oscillator circuits by the coaxial cable reactance. The advance of long distance remote operation inside a vacuum chamber for distances of 45 and 60 m was made possible without altering the quadrupole's rf/dc generator circuit by employing an rf link to drive the quadrupole rods. Applications of the system have been accomplished for in situ space simulation thermal/vacuum testing of sophisticated payloads.			
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## A MODIFIED QUADRUPOLE MASS SPECTROMETER WITH CUSTOM RF LINK RODS DRIVER FOR REMOTE OPERATION

### INTRODUCTION

The quadrupole residual gas analyzer (RGA) is a Process Analyzers, Inc. (PAI) Model 250A nude head system (Fig. 1). The PAI quadrupole RGA [1-6] uses a group of four circular, rod-shaped electrodes with the superimposed dc and rf voltages balanced about ground (Fig. 2). These dc and rf potentials function together to provide the filtering action. Thus, only ions with a specific mass-to-charge ratio reach the detector. This occurs because ions of heavier and lighter masses do not physically oscillate in the electric fields with the correct resonant frequency and amplitude and are deflected away from the quadrupole's axis to be neutralized on the rods. Operation inside a vacuum chamber for the standard quadrupole nude head is limited to approximately 2 m from its externally located rf/dc generator because of the detuning of the rf oscillator circuits by the coaxial cable reactance.

It became necessary in mid-1971 to extend the operating distance of the quadrupole RGA to 45 m because of the need for monitoring NASA's Apollo Telescope Mount (ATM) which was undergoing thermal vacuum testing in the Johnson Spacecraft Center's (JSC) Vacuum Chamber A at Houston, Texas. The ATM, a part of NASA's Skylab and Orbital Workshop Space Station (Fig. 3), is a manned solar observatory which is capable of observing, monitoring, and recording the structure and behavior of the sun. It has been recognized from previous optical flight experiments that the vacuum chamber as well as the ATM may be a source of optical contamination which could degrade the ATM optical experiments through scattering of signals and deposition onto critical surfaces. The objective of monitoring with the quadrupole RGA inside Chamber A was to verify that the chamber, the ATM and its associated systems, and the vehicle support equipment would not be sources of contamination to the ATM optical instruments.

## TEST DESCRIPTION

Chamber A is a stainless steel vacuum chamber 20 m in diameter and 36 m high. Figure 4 shows Chamber A with the ATM mounted in the sun-up position. Above and to the right of the ATM is the quadrupole RGA, mounted on the Naval Research Laboratory's (NRL) Real Time Contamination Monitor (RTCM). The RTCM was designed by William R. Hunter of NRL to measure the changes in reflectance of a mirror surface at 121.6 nanometers (1216 Å), the Lyman-alpha line of hydrogen. Figure 5 is a closeup view of the two instruments. Chamber A [7] provided a base pressure of  $1 \times 10^{-6}$  torr and thermal solar radiation adequate for transient and steady state heat transfer studies and design verification tests performed on the ATM. Figure 6 shows the quadrupole RGA and the RTCM mounted underneath the ATM aperture doors for the ATM sun-end-down phase of the test.

## THEORY OF OPERATION

The quadrupole RGA is an electric quadrupole mass filter of the type invented by Paul [2]. An ion beam is injected along the axis of the head which consists of four matched precision rods approximately 0.1 m long and 0.01 m in diameter. The rods [1] are precisely located in a rectangular array by a matched pair of alumina insulators which support them. Using the design equations by Paul [2] it can be shown that when a dc voltage  $U$  with a superimposed rf voltage  $V_0 \cos \omega t$  is applied across the four parallel rods [3, 8], the potential  $\Phi$  of the field is given by

$$\Phi = (U + V_0 \cos \omega t) \left( \frac{x^2 - y^2}{r_0^2} \right) \quad (1)$$

where the distance between the rods is  $2r_0$ , and  $r_0$  is equal to 0.003 m for the PAI quadrupole RGA.

The motion of an ion having a specific charge-to-mass ratio,  $e/m$ , injected parallel to the  $z$ -axis can be expressed by the following equations:

$$\ddot{x} + \frac{2e}{m r_0^2} (U + V_0 \cos \omega t) x = 0 \quad , \quad (2)$$

$$\ddot{y} - \frac{2e}{m r_0^2} (U + V_0 \cos \omega t) y = 0 \quad , \quad (3)$$

$$\ddot{z} = 0 \quad . \quad (4)$$

Equations (2) and (3) [2, 4] are known as Mathieu's differential equations and describe the oscillations of an ion under the influence of a periodic force. Equation (4) [2] shows that ions injected in the z-direction move through the field in that direction at constant speed.

By using the transformation parameters

$$\left. \begin{aligned} \omega t &= 2\rho \\ a &= \frac{8eU}{m r_0^2 \omega^2} \\ q &= \frac{4eV_0}{m r_0^2 \omega^2} \end{aligned} \right\} , \quad (5)$$

the orthogonal [3] set of equations in x and y become

$$x'' + (a + 2q \cos 2\rho) x = 0 \quad (6)$$

$$y'' - (a + 2q \cos 2\rho) y = 0 \quad (7)$$

where the primes denote differentiation with respect to  $\rho$ .

The general solutions [2, 3, 6, 9] of equations (6) and (7) show that the amplitude of the ions as they traverse the filter either is bounded and oscillates between zero and a maximum value or grows exponentially with time. These oscillations remain below a maximum amplitude only for certain values of the parameters  $a$  and  $q$ . A stability diagram can be constructed which determines the range of  $a/q$  values that are consistent with a real solution.

The theoretical resolution [2, 10] for the quadrupole RGA is given by

$$\frac{m}{\Delta m} = \frac{0.126}{0.16784 - U/V} \quad (8)$$

where the slope of the line of the stability diagram is given by  $a/q$  and, therefore,  $U/V$ . One can immediately determine from equation (8) that the resolution can be changed by varying the ratio  $U/V$  and that theoretical infinite resolution can be achieved for  $U/V = 0.16784$ . In practice, the resolution is altered by reducing the slope  $U/V < 0.16784$ . Decreasing the ratio lowers the resolution. Conversely, as one approaches the  $U/V$  ratio of 0.16784, the transmission of ions decreases drastically, i.e., as resolution increases, sensitivity decreases. In the normal mode of operation for the PAI quadrupole RGA, the ratio of the dc to rf voltages remains constant near the theoretical limit of 0.16784.

## INSTRUMENT REQUIREMENTS

The rf/dc generator [2, 3] in the electronics console of a quadrupole mass spectrometer supplies the proper voltages to the filter rods. The ratio of the dc and rf voltages thus provided determines both the resolution and the sensitivity of the instrument. Holding this ratio precisely constant as a sawtooth sweep voltage is applied was a primary requirement. The dc and rf voltages increase from 0 to 200 Vdc and from 0 to 2400 V peak to peak, respectively. As this voltage ramp is increased, ions are accepted and transmitted through the quadrupole mass filter in order of increasing mass or  $m/e$  value. Even a small change in the dc/rf ratio, which is difficult to maintain during cable extension, produces a large change in the quadrupole system resolution and sensitivity. In addition, this vacuum application required the PAI quadrupole RGA to be operated at near maximum resolution. Small deviations in the dc/rf values in this region of the stability diagram would lead to a small change in resolution but a large decrease in ions transmitted through the filter to the detector; i.e., sensitivity.

The quadrupole RGA rf/dc generator was set up for the mass range of 10 to 250 amu which occurs for a system frequency of 3.3 MHz. The quadrupole sensor head functions as a capacitor [2,3,4] and shunts the rf/dc generator tank circuit. Thus, any increase in cable length; i.e.,



capacitance, detunes the circuit, and the resonance frequency (3.3 MHz) shifts because of its LC product dependence. Avoiding this detuning effect while implementing the modification steps was a second requirement. A third requirement was the assurance of maximum power transfer from the electronics console to the quadrupole head.

As with most test or research applications, there were additional constraints or requirements. Principal among these was the necessity to assure that there were no spurious effects on other instrumentation. For example, the rf link system should not generate electromagnetic interference (EMI) of any type, and it should not functionally cause unnecessary reflections or oscillations of either dc or rf power in the circuitry. Of course, a final requirement is that the general modification approach should be demonstrably applicable, with the appropriate changes in details, to other commercial designs of quadrupole mass spectrometers.

## RF LINK RODS DRIVER

The most critical instrument requirement is maintenance of an accurate and stable dc/rf ratio (one part in  $10^5$ ), once it has been established for a maximum overall filter effectiveness as evidenced by high sensitivity and good resolution. Therefore, one first selects a frequency within the range of the system tuning capacitor. Next, the rf potential to each end of the rf/dc generator tank coil is balanced (usually by a "butterfly" capacitor). The only variable remaining is the value of the dc to be imposed for a given rf peak voltage at a given time. This applies whether the mode of operation is manual, automatic, or programmed. The adjustment for this last parameter is in the peaking capacitors for the ramp voltage outputs located in the rf/dc generator. The rf voltage ramp for scanning should be very smooth to preserve the rf/dc ratio. This is assured by sending to the modulator driver the rf sampled from each end of the rf/dc generator tank coil (Fig. 7). The criterion is that the rf level at the rf tank output be free of random variations in amplitude.

Large cable lengths are added to the above conditions. This means that the capacity of the coaxial cables (or even open line cabling) loads the rf tank and makes ramp stability and smoothness for a selected frequency unlikely. To overcome the capacitive loading problem, it was decided to

inductively couple the power by a long coaxial cable to a point (rf link box) which was a short distance from the quadrupole filter rods assembly. The cable, or rf transmission line, to the rf link box was not small compared to the wavelength of the selected range frequency (3.3 MHz). In addition, a requirement to eliminate sources of EMI was assumed. Therefore, it was decided to treat the rf transmission line problem with flat transmission line (ideal) methods as well as to use inductive link coupling [9] (Fig. 8). The rf transmission line and coils should, in general, be set up for impedance-to-reactance matches. In this particular case, a  $62\text{-}\Omega$  coaxial cable was used. Therefore, by using a grid dipmeter, impedance meter, and coil diameter and properties tables, the rf link box coupling (load coupling) and the rf/dc generator link coil were essentially designed, developed, and/or adjusted to assure a match of  $62\text{ }\Omega$  for the reactances of the coupling coils at 3.3 MHz. The steps of the above technique are considered general knowledge, and the only comment is evidently that this can be done for the particular quadrupole system frequency and reactance. The authors consider the above procedure to virtually assure a flat rf transmission line condition. With the above matched system, the rf transmission line approaches a resistive impedance; therefore, the rf/dc generator adjustments approach independence of cable length. This means that the circuit detuning problem associated with increased cable lengths is avoided.

The next phase is to develop the rf link box. At the rf link box, the transmission line voltage was stepped up to high rf level by a balanced-to-ground rf tank coil. This rf voltage was applied to the appropriate rod pair by a 1- to 2-m rf line. The synchronized dc ramp voltage was applied directly to the appropriate rod pair by a shunt circuit. The rf link box tank coil was isolated to prevent EMI and other disturbances by rf chokes, and the rf link box tank coil electrical center (grounded to be at the same potential as the quadrupole head) was protected from dc voltages by dc blocking capacitors. Several solutions to rf transmission line and rf link problems are possible. However, the inherent nature of the RGA power transmission and maintenance situation as well as the problems associated with in situ operation seem to dictate that the best approach is the simplest one. Therefore, the rf link box tank coil and its rf link coil (coupling coil) were permanently wound and mounted with tight coupling to insure a constant stepping-transformer system. The one-piece rf tank coil assured symmetry and eliminated alignment problems. The rf link coil (Fig. 9) satisfied a minimum condition (two turns) and avoided the necessity for complex in situ mechanical control and stability of variable coupling. The geometry of the rf chokes and dc stopping capacitors assured minimal extraneous voltage

paths and, thus, minimum interference. A consideration away from the mechanically clean approach could involve the use of a "butterfly" balancing capacitor for the rf link box—perhaps controlled by a vacuum-rated stepping motor. This would add extra control to assure that precise rf voltage values were being applied to the appropriate filter rod pairs; however, development time did not permit this. Within the range of measurement by rf probes and dual-beam oscilloscope, it was determined that the rf potentials were delivered in satisfactory balance (Fig. 10). This meant that the dc potentials could be varied at the console to complete the achievement of optimum output; i. e. , resolution and sensitivity maximized.

## TUNING THE SYSTEM

A custom vacuum station for field and remote site use was developed and used to tune and calibrate the PAI quadrupole RGA with the rf link (Figs. 11 and 12) at 45-m separation prior to chamber installation. The test console consists of a heated, dual-inlet system; the sensor head; interconnecting valving gauges; and an ion/sorption pumping system. The sample material used for calibration in this study was Bromoform ( $\text{CHBr}_3$ ).

There are at least three approaches to a detection method for monitoring tuning procedures for this rf link. The first two approaches are recommended for initial coarse phases of adjustments to the electronics console and the rf link. First, a fluorescent tube may be used to visually evaluate the degree of power transfer over the rf transmission line to the rf link box. This is done by placing the lamp near each end of the rf link tank coil in turn while adjustments are varied. Maximizing and balancing of controls are done for each side, with lamp intensity as the evaluation factor. The second method consists of removing the dc voltage from the rods. With the dc/rf ratio at zero, the quadrupole system resolution goes to zero. With no filtering action, all ions reach the detector. This total ion current measurement is a total pressure value which is displayed on the system oscilloscope. Thus, to complete the setup, the rf voltage is increased to the coils until the total pressure curve is maximized; i. e. , an optimum dc/rf balance. Third, the approach for completing the system setup is to fine tune, using a dual-beam oscilloscope with rf probes so that the voltages on each sensing rod can be directly measured, displayed, and matched for exact balance. Then the calibration sample (in this case Bromoform) is introduced, and rf/dc generator adjustments (peaking capacitors) are made for concurrent optimum resolution and sensitivity.

## EXPERIMENTAL AND TEST RESULTS

The described quadrupole RGA system was successfully operated as a qualitative analytical unit in the tests described in the Introduction. The system was stable for the mass range desired, and it met the guidelines set up in the instrument requirements description. The purpose of this project was to establish a capability which did not exist. Thus, success was evaluated by the ability to make measurements and not by any criteria of increasing system accuracy or sensitivity. A photograph of an oscilloscope mass scan display was taken directly from the PAI quadrupole console at a 45-m separation (Fig. 13). The effective mass range displayed was 12 to 180 amu, and the calibration material was Bromoform. The Bromoform molecule has two abundant isotopes, one at mass 79 amu (50.5 percent) and the other at mass 81 amu (49.5 percent). Comparison with a reference spectrum (Fig. 14) showed that all the essential "cracking pattern" information was presented. For quantitative work, there remained an unexplained relative peak height problem between the abundant ions and the  $\text{CHBr}^+$  fragment isotope triplet. Because these methods have been successfully applied to a different RGA system by another NASA group, these descriptions should be applicable by and of value to other researchers.

## SUMMARY

A Process Analyzers, Inc., quadrupole mass spectrometer was upgraded for vacuum chamber test and field applications which require extended cable lengths. Overall, the instrument's operation during the Chamber A tests of the Apollo Telescope Mount provided acceptable mass spectra scans at a separation of 45 m. Colleagues at the Johnson Spacecraft Center have subsequently used these guidelines to successfully upgrade another commercial quadrupole mass spectrometer. With additional design improvements in certain details and sufficient time for subsystem setups, this instrument should also perform quantitatively on a level with systems operating at standard cable length separations.

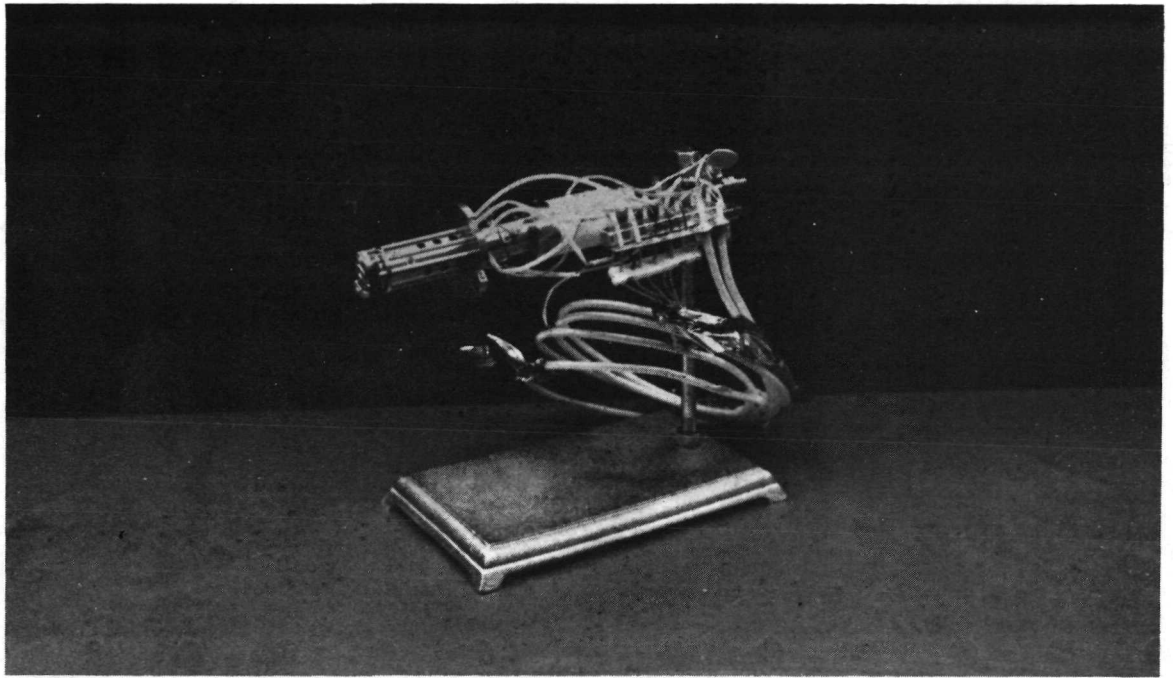


Figure 1. Process Analyzers, Inc. Model 250A quadrupole nude head assembly.

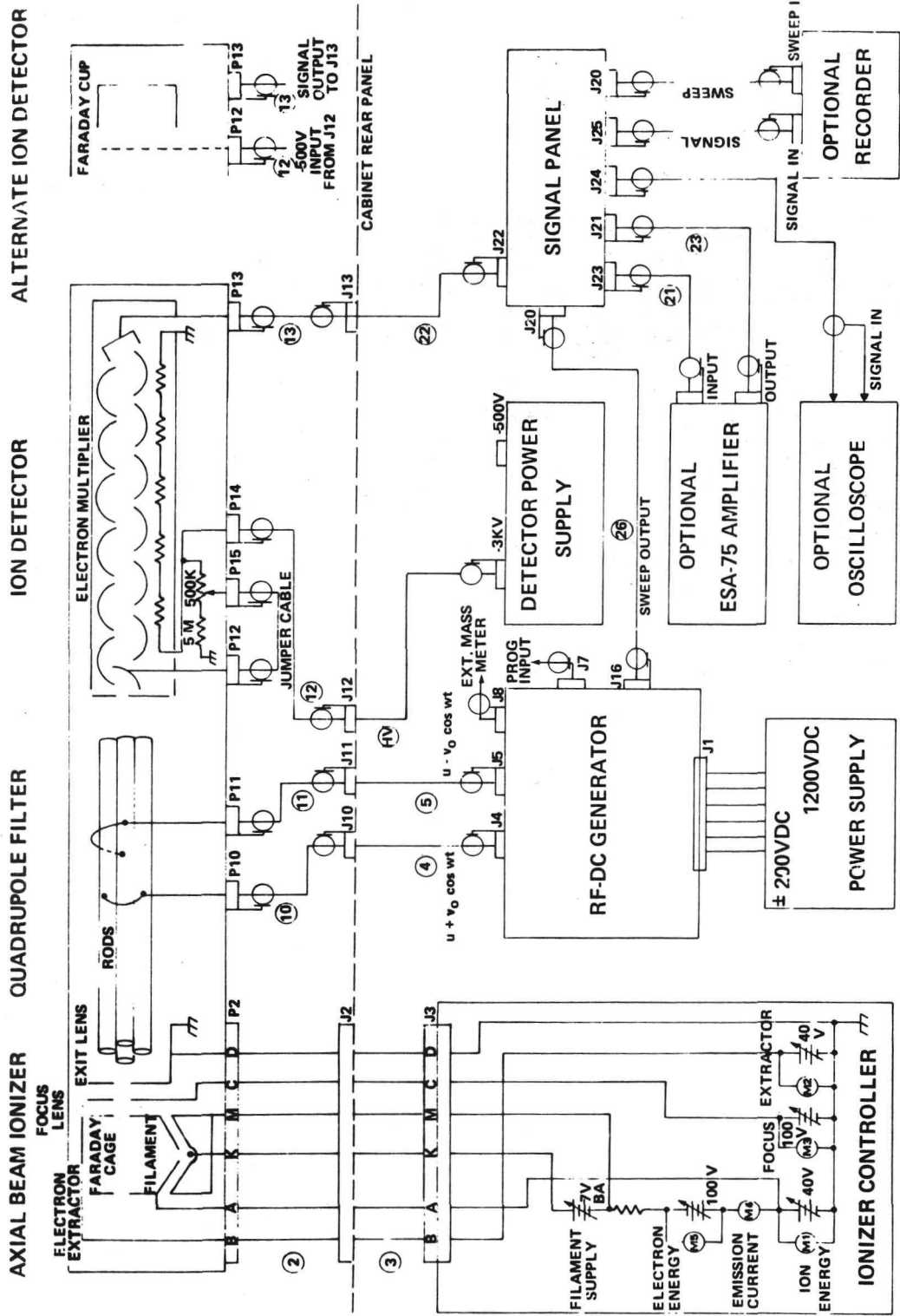


Figure 2. Diagram of PAI quadrupole residual gas analyzer system.

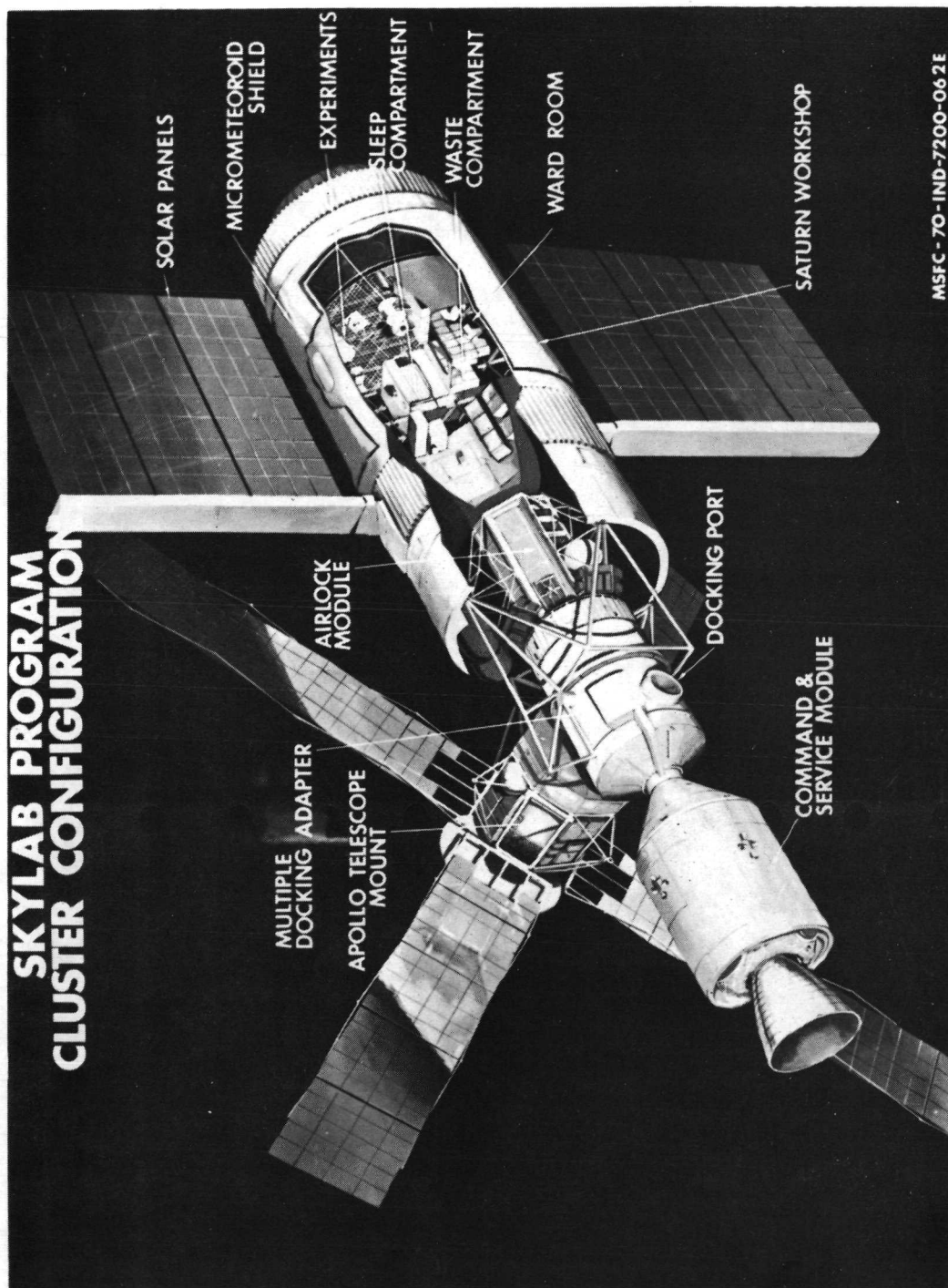


Figure 3. Artist's concept of Skylab hardware flight configuration.

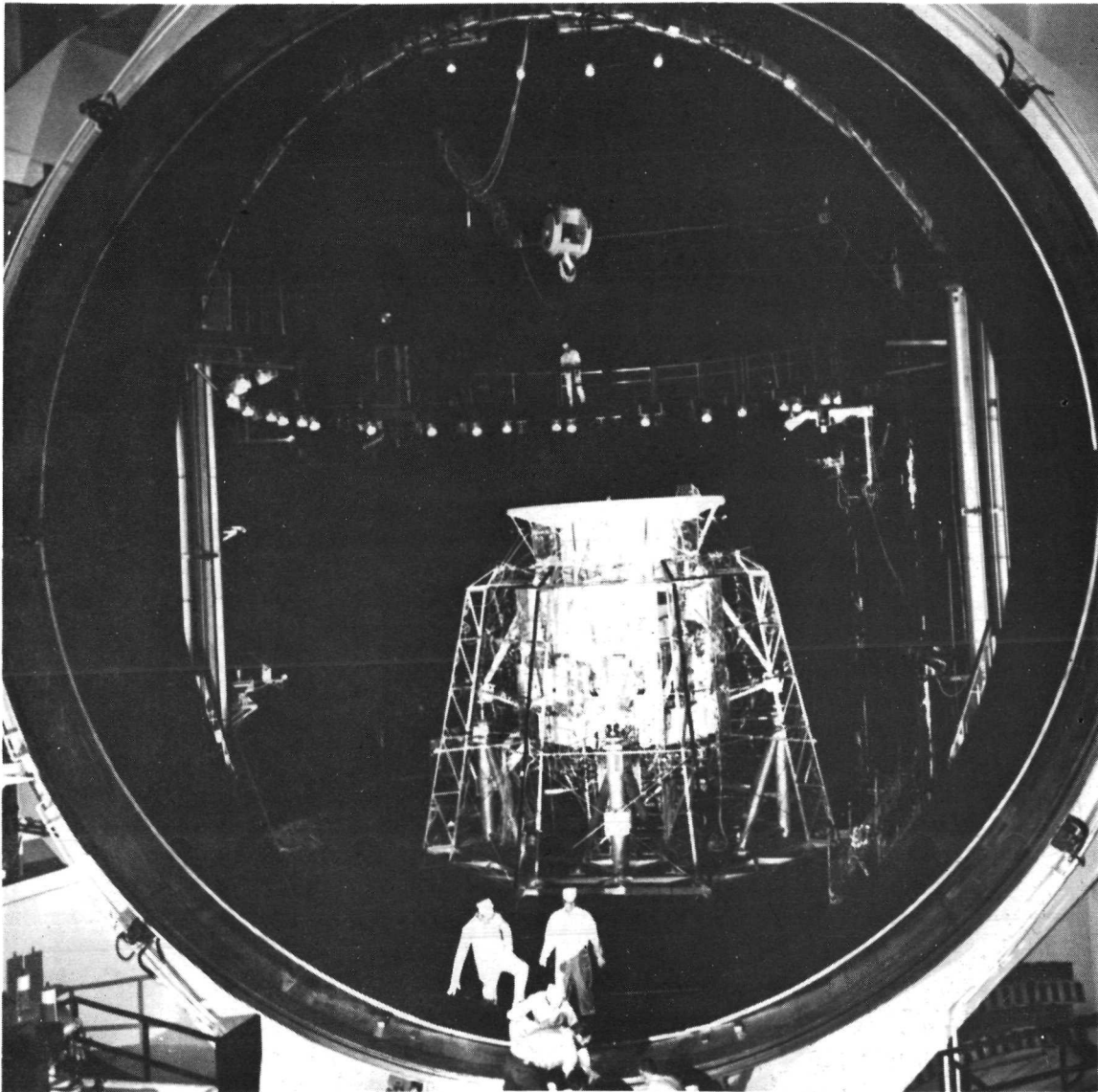


Figure 4. ATM TV-2 Test — Quad RGA, RTCM, QCM and ion gauge viewing the ATM sunshield in JSC Chamber A.



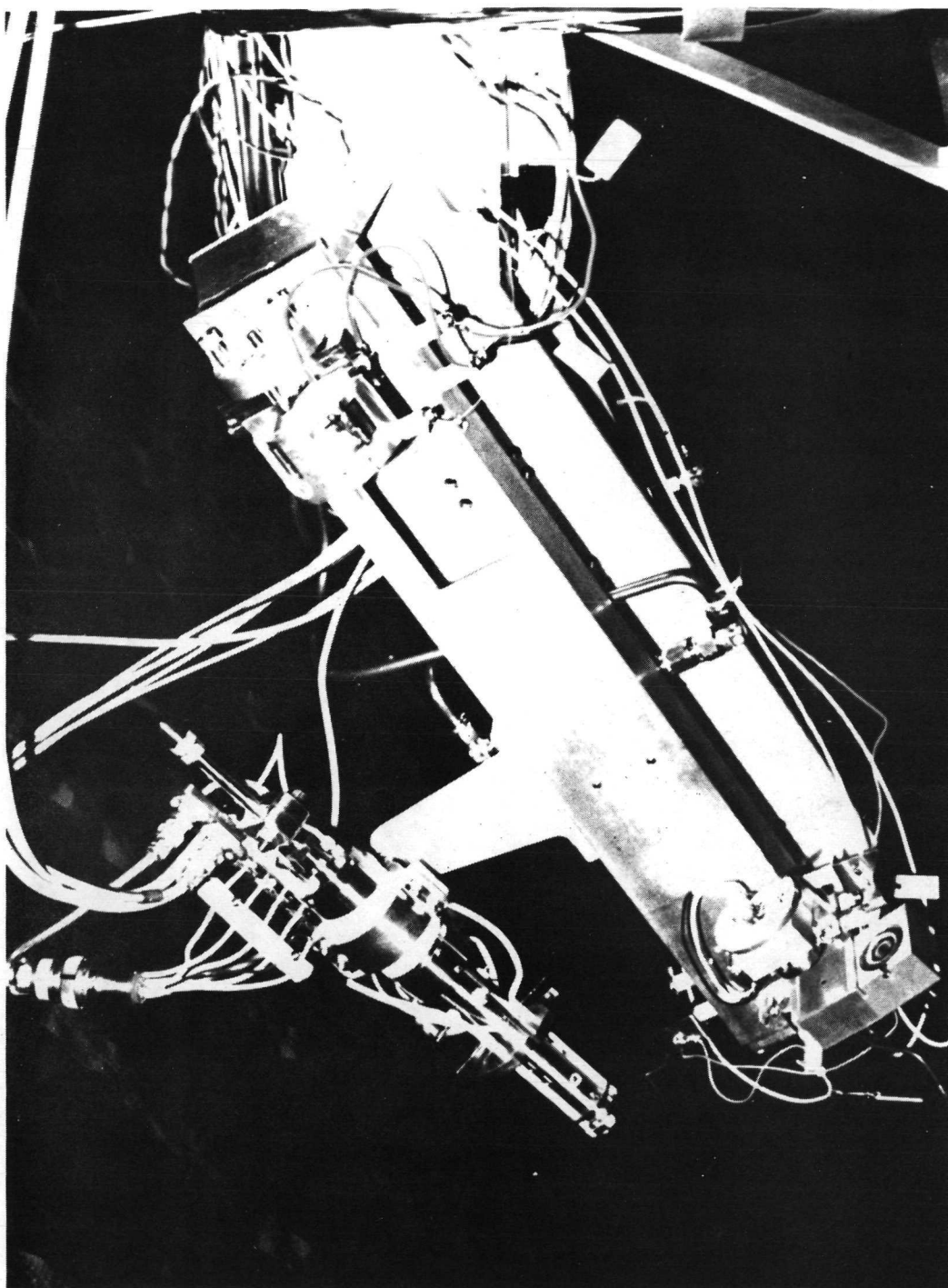


Figure 5. ATM Chamber A test mounting configuration for PAI quadrupole RGA and NRL RTCM.

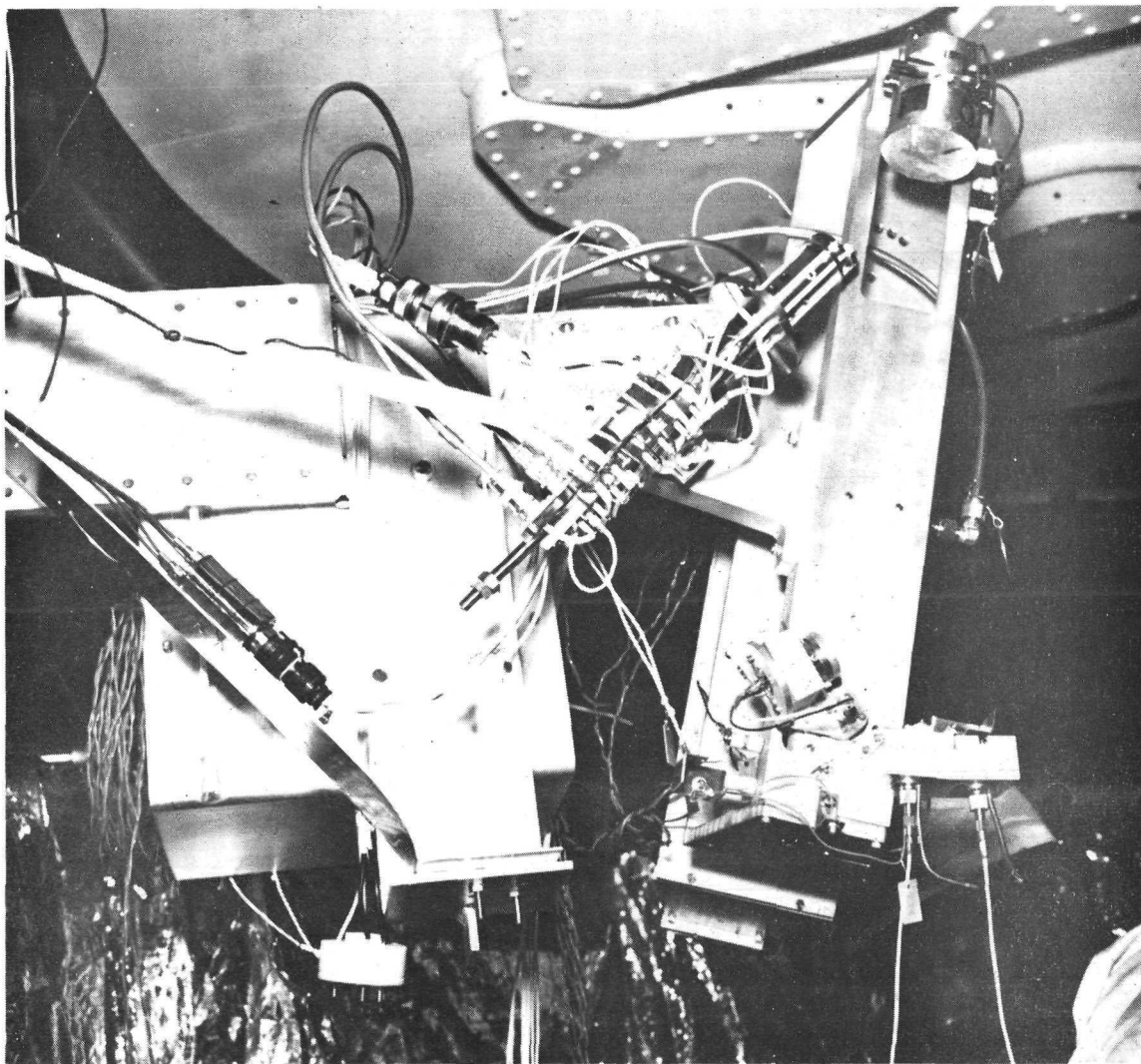


Figure 6. ATM TV-1 Test — PAI quadrupole RGA and ion gauge QCM and NRL RTCM viewing the ATM in the sun-down position.

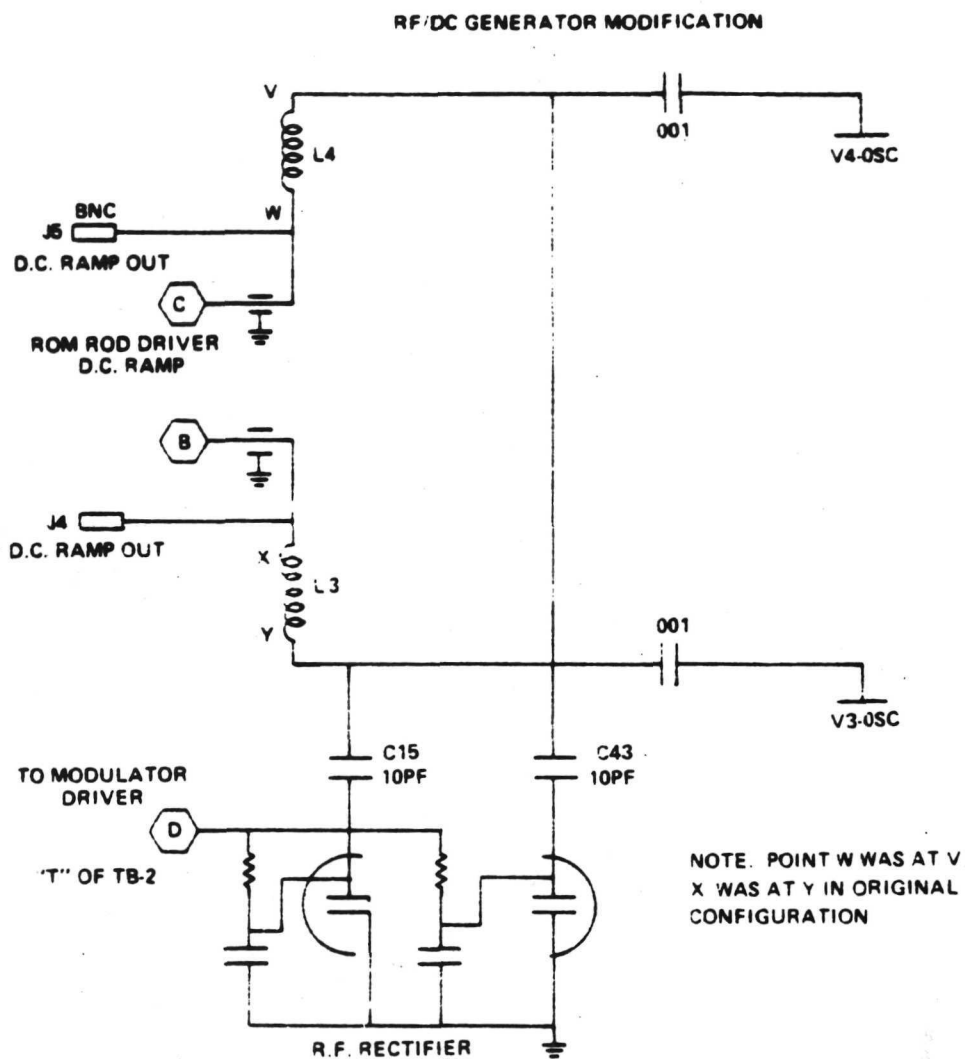


Figure 7. rf/dc generator modification.



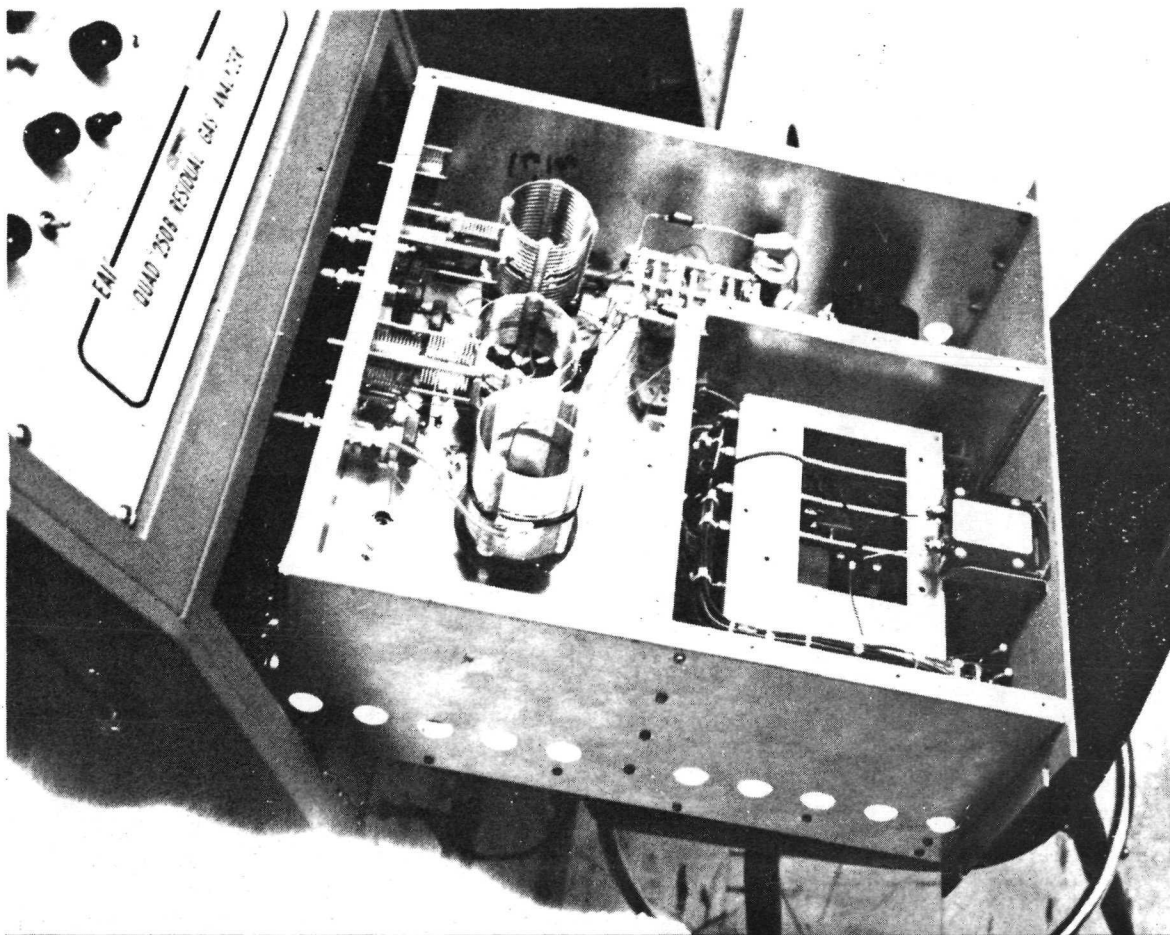


Figure 9. Link coil wound on the rf/dc generator resonant coils  
(center coil utilized).

# R.F. LINK ROD DRIVER (BLACK BOX)

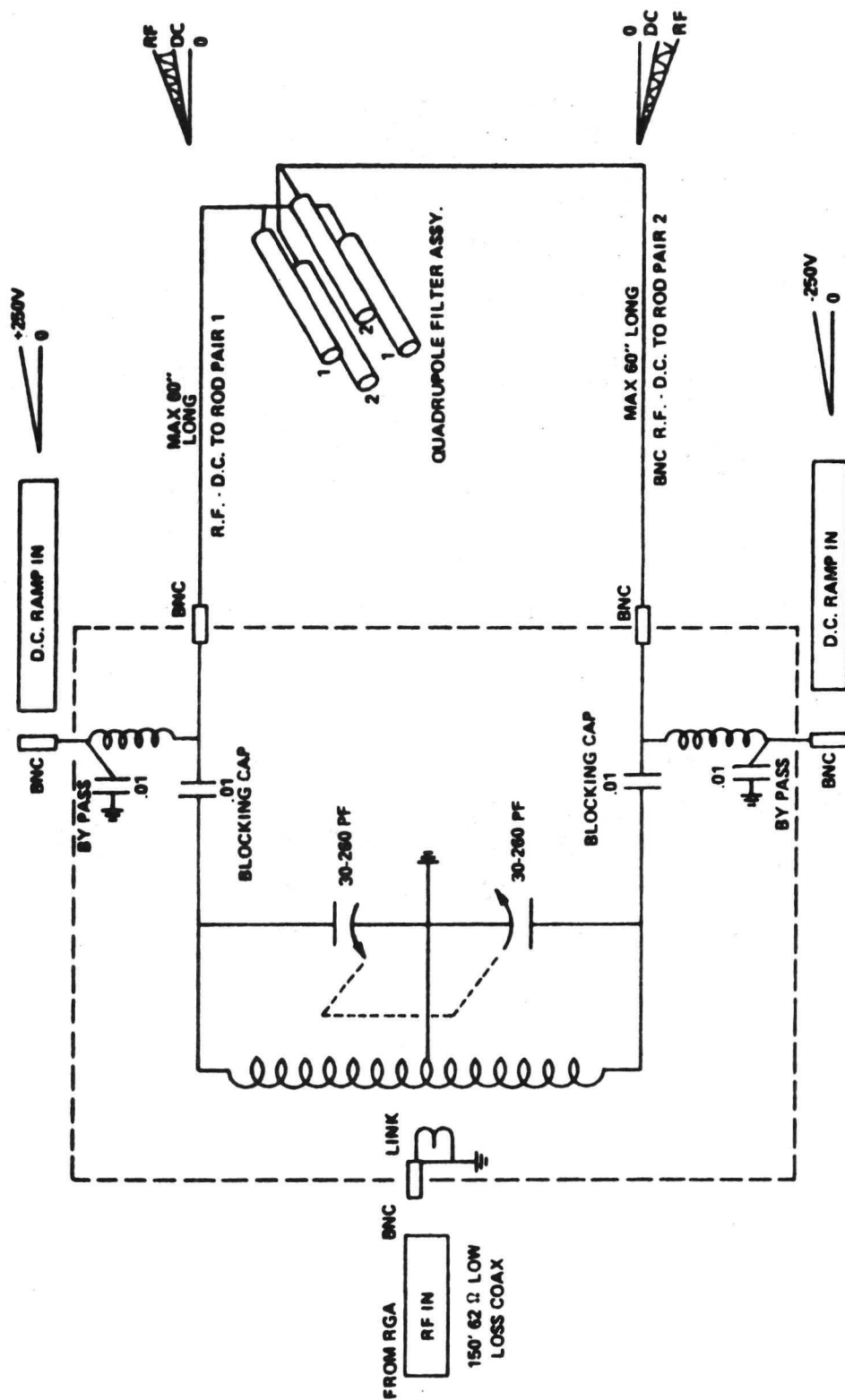


Figure 10. rf link design at the quadrupole head.

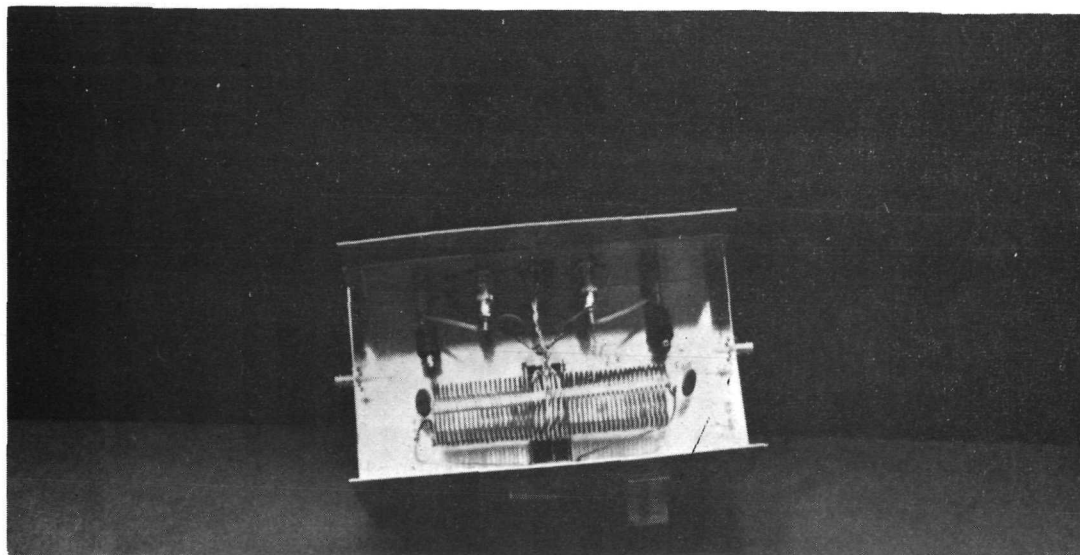


Figure 11. Physical layout of the rf link box.

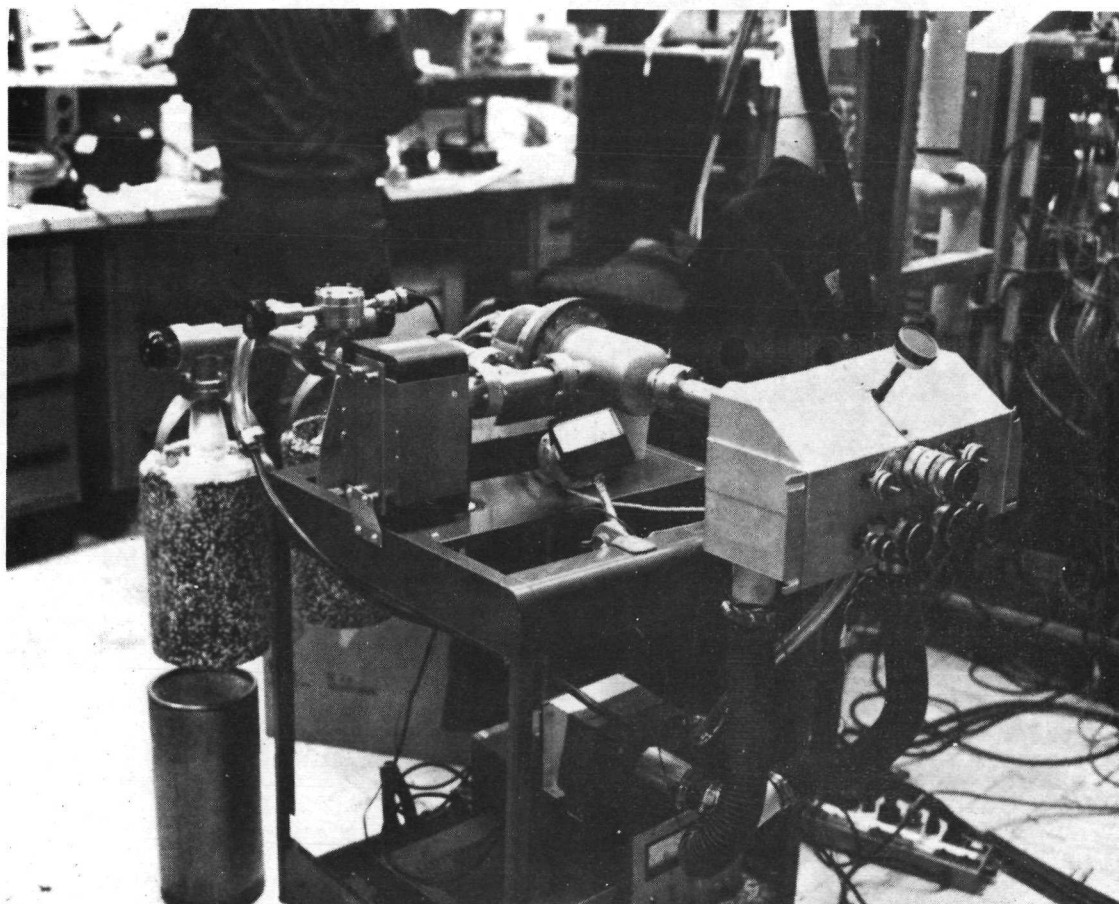


Figure 12. Test console used to calibrate and tune the quadrupole RGA with rf link.



SYSTEM SETTINGS:

ELECTROMULTIPLIER - 1550 volts

PRESSURE -  $4.9 \times 10^{-6}$  torr

RANGE - 10 TO 180 amu

SCOPE VERTICAL - 0.5 V/cm

ION ENERGY - 40 volts

ELECTRONS ENERGY - 70 eV

SCAN TIME - 0.3 sec

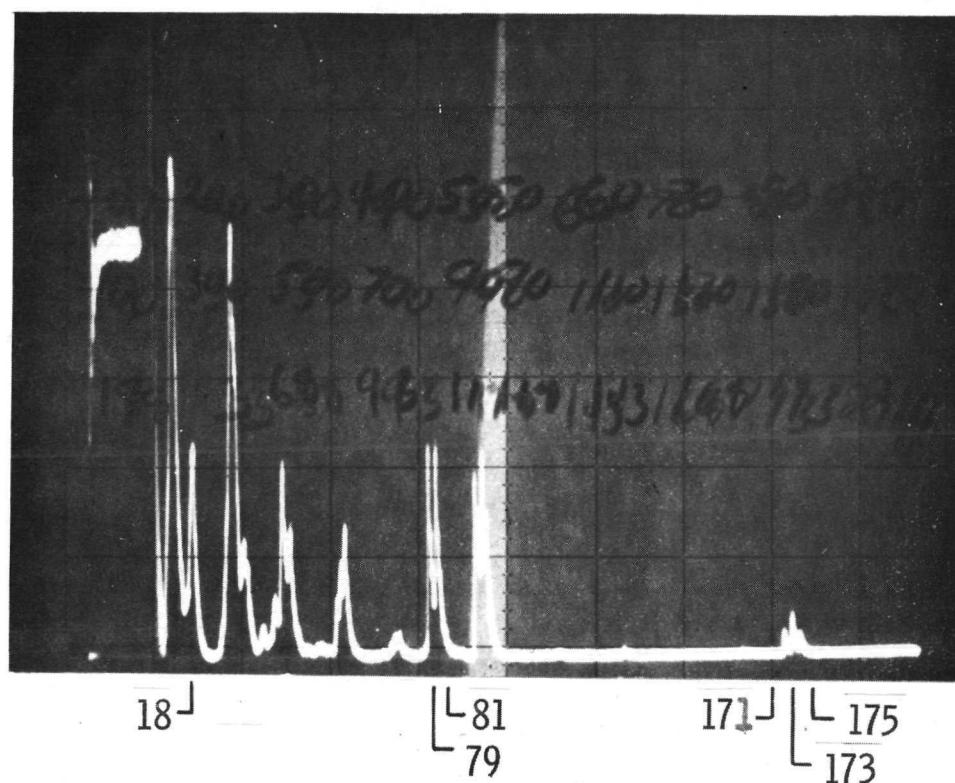


Figure 13. Representative mass scan of Bromoform from PAI quadrupole RGA.



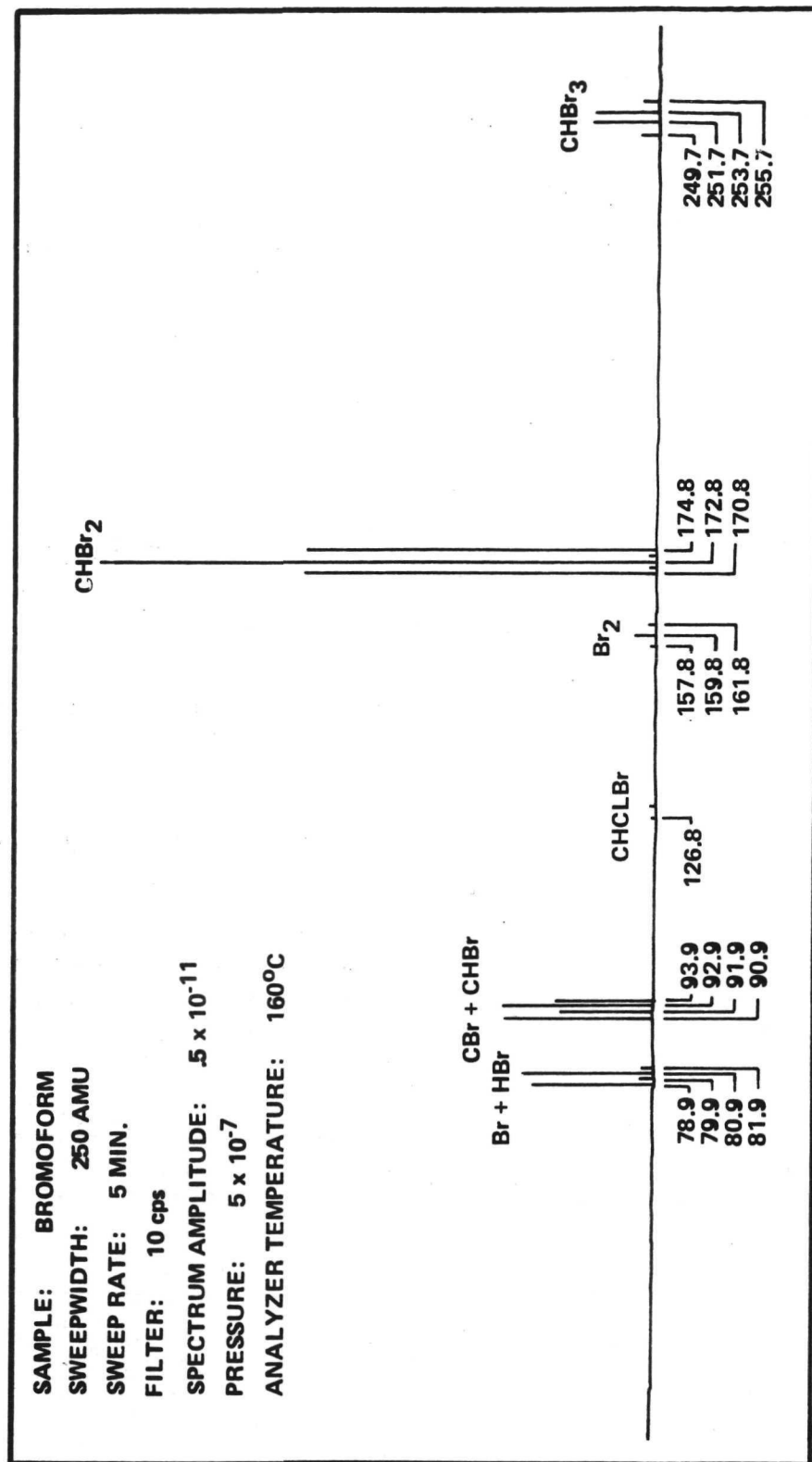


Figure 14. Reference mass spectrometer scan of Bromoform generated by Varian Analytical Instruments M-66 mass spectrometer.

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## APPROVAL

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The information in this report has been reviewed for security classification. Review of any information concerning Department of Defense or Atomic Energy Commission programs has been made by the MSFC Security Classification Officer. This report, in its entirety, has been determined to be unclassified.

This document has also been reviewed and approved for technical accuracy.



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